FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
FACULTY OF ENGINEERING

Performance Engineering of the Kernel Polynomial Method on Large-Scale CPU-GPU Systems

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SPPEXA

Prologue (I)

The **ESSEX** project

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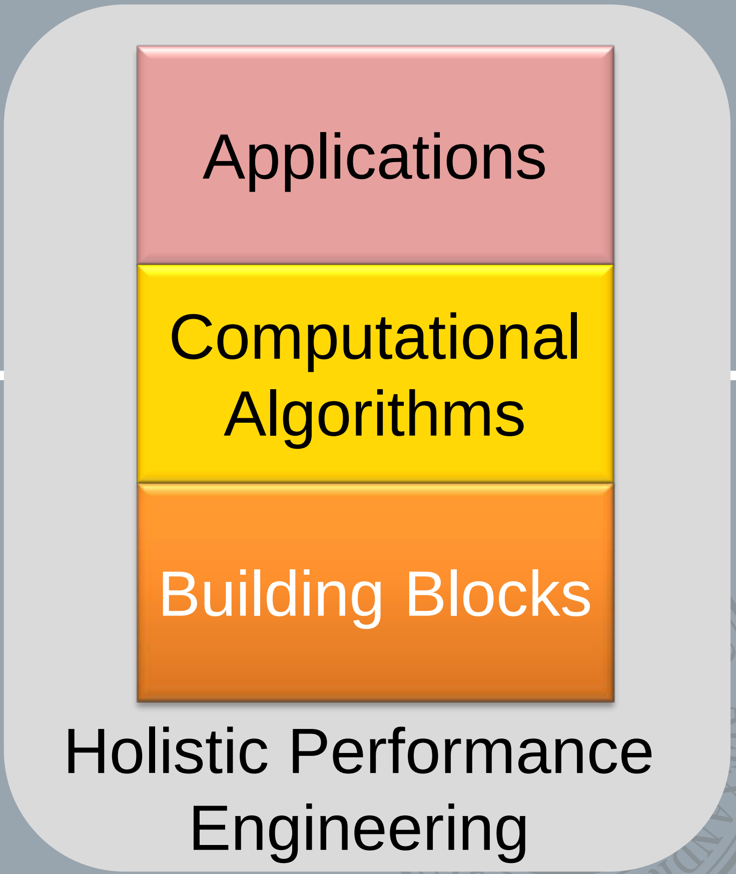


Equipping Sparse Solvers for Exascale: Motivation

Hardware

Fault tolerance
Energy efficiency
New levels of parallelism

Quantum Physics Applications

Extremely large sparse matrices:
eigenvalues, spectral properties,
time evolution

ESSEX

Exascale Sparse Solver Repository (ESSR)

- FT concepts, programming for extreme parallelism
- Sparse eigensolvers, preconditioners, spectral methods
- Quantum physics / chemistry
- ESSEX applications: Graphene, topological insulators, …

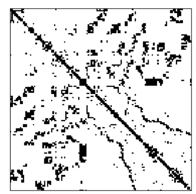
Prologue (II)

What is the **K**ernel **P**olynomial **M**ethod and why heterogeneous computing?

The Kernel Polynomial Method (KPM)

Approximate the complete eigenvalue spectrum of a large sparse matrix.

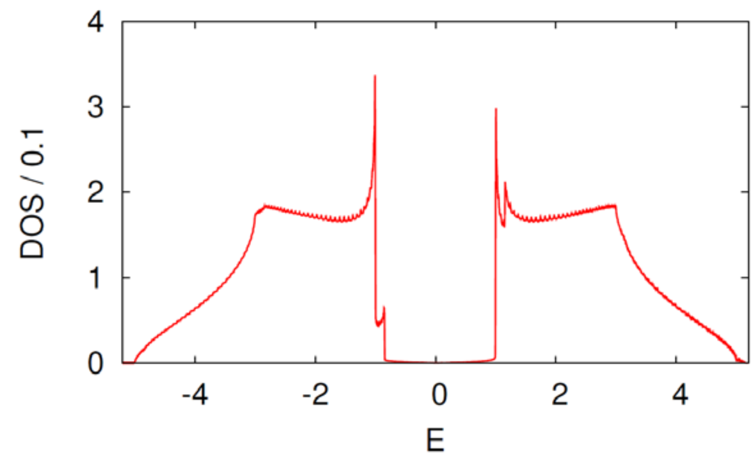
Large, Sparse



$$\boldsymbol{H}\,\boldsymbol{x} = \lambda\,\boldsymbol{x}$$

$$\underbrace{\{\lambda_1, \lambda_2, \dots, \lambda_k, \dots, \lambda_{n-1}, \lambda_n\}}$$

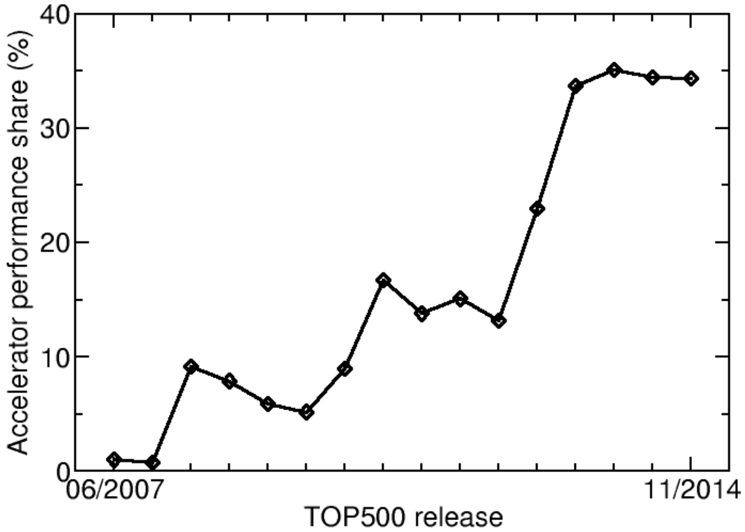
Good approximation to full spectrum
(e.g. Density of States)



A. Weiße, G. Wellein, A. Alvermann, H. Fehske: **"The kernel polynomial method"**, Rev. Mod. Phys., vol. 78, p. 275, 2006.
E. di Napoli, E. Polizzi, Y. Saad: **"Efficient estimation of eigenvalue counts in an interval"**, Preprint. http://arxiv.org/abs/1308.4275
O. Bhardwaj, Y. Ineichen, C. Bekas and A. Curioni.: "**Highly scalable linear time estimation of spectrograms - a tool for very large scale data analysis**", SC13 Poster.

Why optimize for heterogeneous systems?

One third of TOP500 performance stems from accelerators.



But: **Few <u>truly</u> heterogeneous software.**

(Using both CPUs and accelerators.)

The Kernel Polynomial Method

Algorithmic Analysis

The Kernel Polynomial Method

Compute Chebyshev polynomials and moments.

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

Holistic view: Optimize across all software layers!

Building blocks: (Sparse) linear algebra library

for $r = 0$ to $R-1$ **do** — **Application**: Loop over random initial states

$\quad |v\rangle \leftarrow |\mathrm{rand}()\rangle$

$\quad$ Initialization steps and computation of η_0, η_1

$\quad$ **for** $m = 1$ to $M/2$ **do** — **Algorithm**: Loop over moments

$\quad\quad \mathrm{swap}(|w\rangle, |v\rangle)$

$\quad\quad |u\rangle \leftarrow H|v\rangle$ — ▷ spmv()

$\quad\quad |u\rangle \leftarrow |u\rangle - b|v\rangle$ — ▷ axpy()

$\quad\quad |w\rangle \leftarrow -|w\rangle$ — ▷ scal()

$\quad\quad |w\rangle \leftarrow |w\rangle + 2a|u\rangle$ — ▷ axpy()

$\quad\quad \eta_{2m} \leftarrow \langle v|v\rangle$ — ▷ nrm2()

$\quad\quad \eta_{2m+1} \leftarrow \langle w|v\rangle$ — ▷ dot()

$\quad$ **end for**

end for

- 1 **do**

steps and computation of η_0, η_1

$M/2$ **do**

$, |v\rangle)$

$(H - b\mathbb{1})|v\rangle - |w\rangle$ &

$= \langle v|v\rangle$ &

$= \langle w|v\rangle$ — ▷ aug_spmv()

▷ aug_spmmv()

Augmented Sparse Matrix Vector Multiply

Augmented Sparse Matrix Multiple Vector Multiply

Dot Product

Analysis of the Algorithmic Optimization

- **Minimum code balance of vanilla algorithm:**
  complex double precision values, 32-bit indices, 13 non-zeros per row, application: topological insulators

$$B_{vanilla} = 3.39\ Bytes/Flop$$ (B = inverse computational intensity)

- **Identified bottleneck: Memory bandwidth**
  ➔ Decrease memory transfers to alleviate bottleneck

- **Algorithmic optimizations reduce code balance:**

$$B_{aug\_spmv} = 2.23\ \ B/F$$ kernel fusion

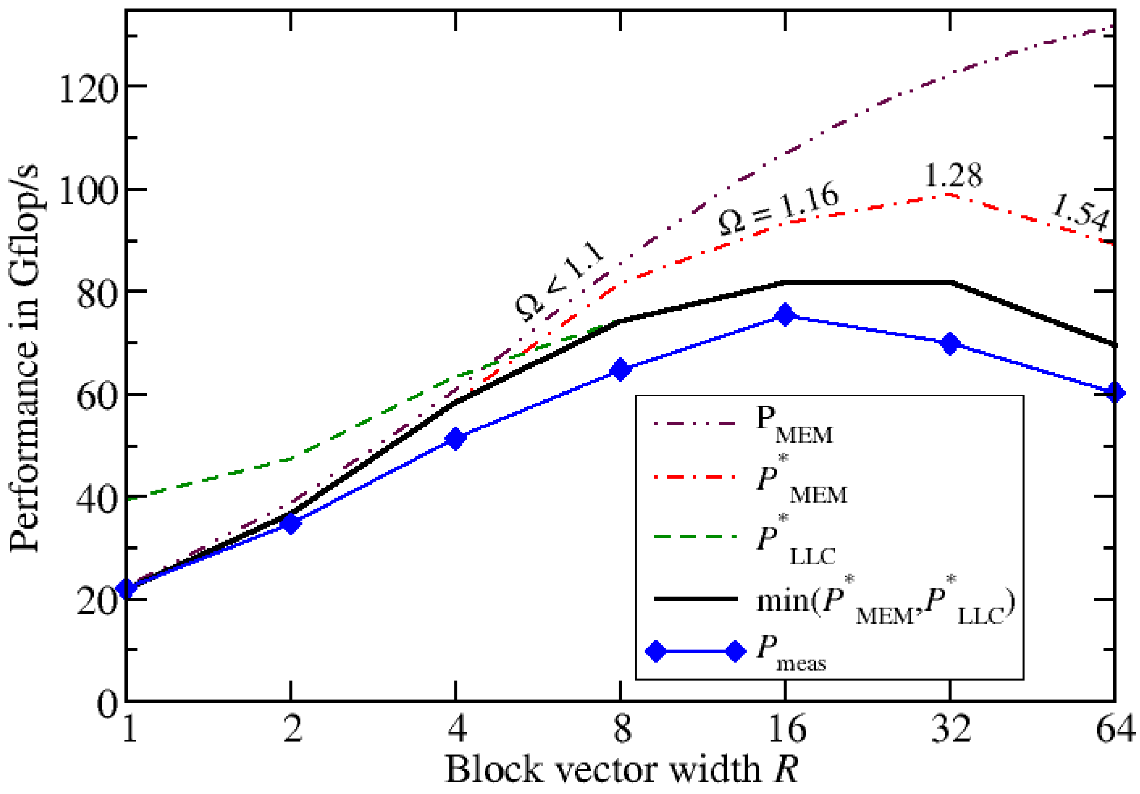
$$B_{aug\_spmmv}(R) = 1.88/R + 0.35\ \ B/F$$ put *R* vectors in block

See also: W. D. Gropp, D. K. Kaushik, D. E. Keyes, and B. F. Smith, "**Towards realistic performance bounds for implicit CFD codes**," in Proceedings of Parallel CFD99. Elsevier, 1999, p. 233.

Consequences of Algorithmic Optimization

- **Mitigation of the relevant bottleneck**
  ➔ Expected speedup
- **Other bottlenecks become relevant**
  ➔ Achieved speedup may not be $B_{vanilla}/B_{aug\_spmmv}$
- **Block vectors are best stored interleaved**
  ➔ May impose larger changes to the codebase
- **`aug_spmmv()` no part of standard libraries**
  ➔ Implementation by hand is necessary

CPU roofline performance model



$P = \frac{b}{B}$ **Gflop/s**

→ Performance limit for bandwidth-bound code

b = max. bandwidth = 50 GB/s
B = code balance

$\Omega = \frac{\text{Actual data transfers}}{\text{Minimum data transfers}}$

S. Williams, A. Waterman, D. Patterson: **"Roofline: An insightful visual performance model for multicore architectures"**, *Commun. ACM*, vol. 52, p. 65, 2009.

Implementation

How to harness a heterogeneous machine in an efficient way?

Implementation

Algorithmic optimizations lead to a *potential* speedup.

➔ We “merely” need an efficient implementation!

Data or task parallelism?

- **MAGMA: task parallelism between devices**
  `http://icl.cs.utk.edu/magma/`
- **Kernel fusion Task parallelism**

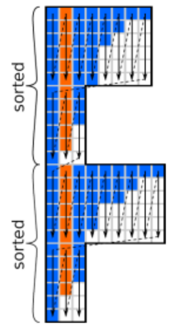
➔ Data-parallel approach suits our needs

Implementation

Data-parallel heterogeneous work distribution

- Static work-distribution by matrix rows/entries
- Device workload ←→ device performance

SELL-C-σ sparse matrix storage format



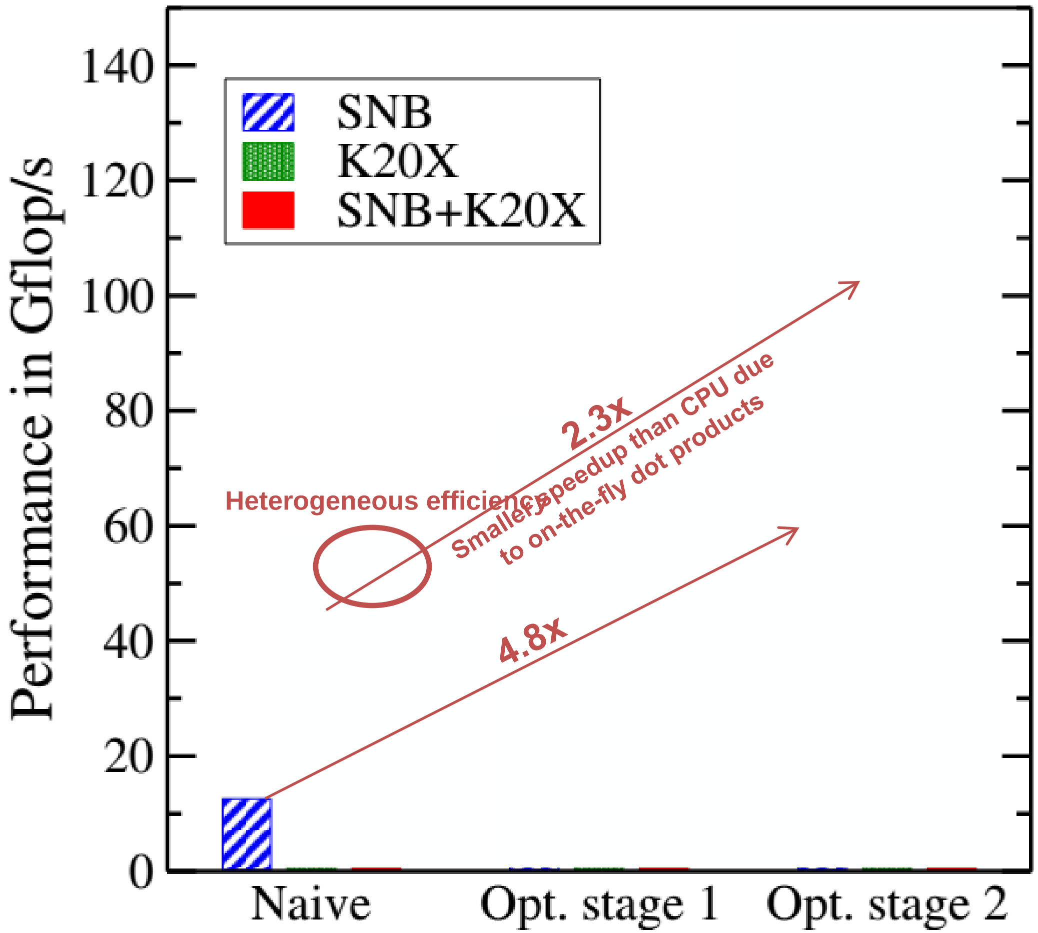
- Unified format for all relevant devices (CPU, GPU, Xeon Phi)
- Allows for runtime-exchange of matrix data (dynamic load balancing, future work)

M. Kreutzer, G. Hager, G. Wellein, H. Fehske, A. R. Bishop, **"A unified sparse matrix data format for efficient general sparse matrix-vector multiplication on modern processors with wide SIMD units"**, *SIAM J. Sci. Comput.*, vol. 36, p. C401, 2014

Performance results

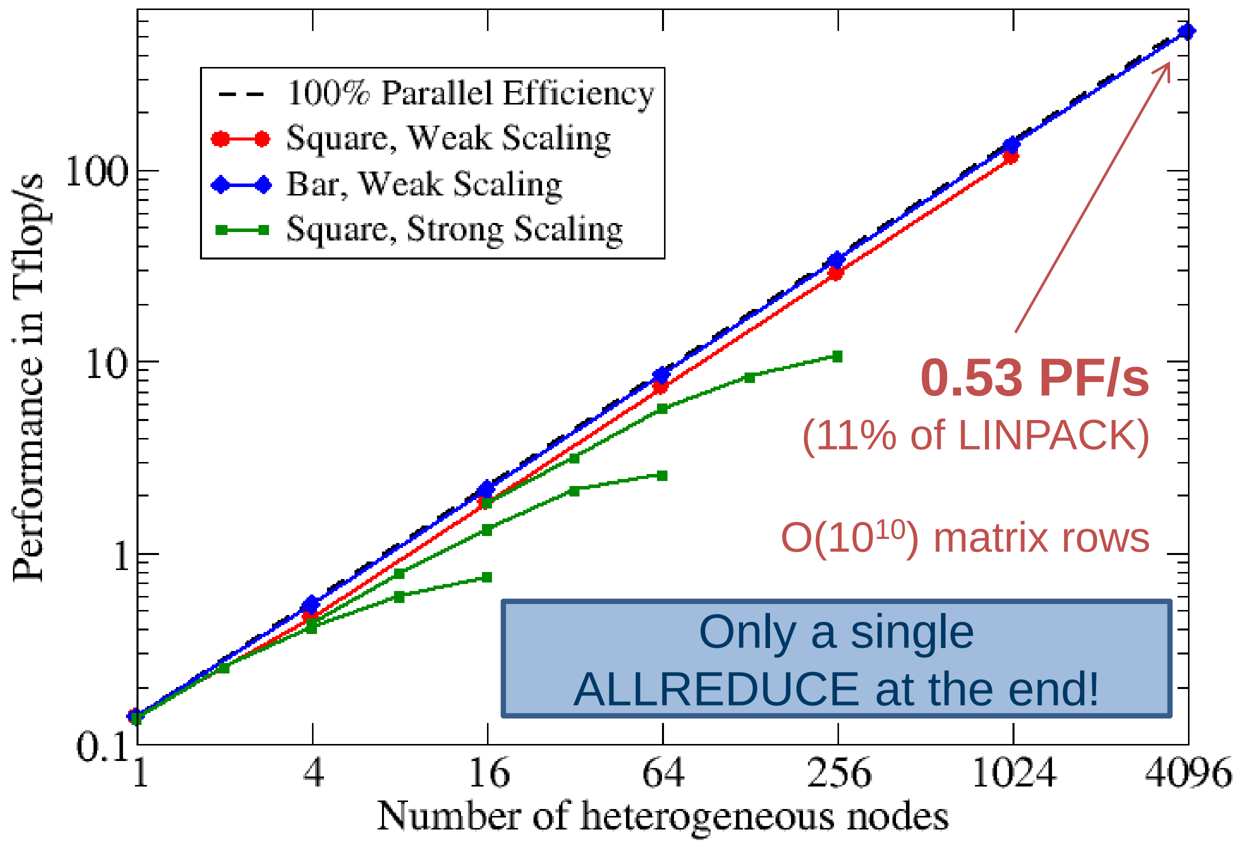
Does all this really pay off?

Single-node Heterogeneous Performance



SNB: Intel Xeon Sandy Bridge, K20X: Nvidia Tesla K20X, Complex double precision matrix/vectors (topological insulator)

Large-scale Heterogeneous Performance



CRAY XC30 – Piz Daint*

- **5272 nodes**, each w/
  - 1 Intel Sandy Bridge
  - 1 NVIDIA K20x

- **Peak: 7.8 PF/s**
- **LINPACK: 6.3 PF/s**

- Largest system in Europe

*Thanks to CSCS/O. Schenk/T. Schulthess for granting access and compute time

Epilogue

Try it out! (If you want...)

Download our building block library & KPM application: http://tiny.cc/ghost

General, Hybrid, and Optimized Sparse Toolkit

- MPI + OpenMP + SIMD + CUDA
- Transparent data-parallel heterogeneous execution
- Affinity-aware task parallelism (checkpointing, comm. hiding, etc.)
- Support for block vectors
  - Automatic code generation for common block vector sizes
  - Hand-tuned tall skinny dense matrix kernels
- Fused kernels (arbitrarily "augmented SpMMV")
- SELL-C-σ heterogeneous sparse matrix format
- Various sparse eigensolvers implemented and downloadable

. . .

ESSEX project webpage: http://blogs.fau.de/essex/

Backup Slides

Only in the unlikely case I was too fast...

Conclusions

- Model-guided performance engineering of KPM on CPU and GPU
- Decoupling from main memory bandwidth
- Optimized node-level performance
- Embedding into massively-parallel application code
- Fully heterogeneous peta-scale performance for a sparse solver

Outlook

- Applications besides KPM
- Automatic (& dynamic) load balancing
- Optimized GPU-CPU-MPI communication
- Further optimization techniques (cache blocking, ...)
- Performance engineering for Xeon Phi (already supported